Animated simulation of the paths of the wave fields in a crystal containing a dislocation

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11.7-1 ANIMATED SIMULATION OF THE PATHS OF THE WAVE FIELDS IN A CRYSTAL CONTAINING A DISLOCATION. by

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Simulation allows to simulate the contrast of a defect in X- Ray topography. It may also be used to understand the interaction between the wavefields and the deformed crystal in a plane of incidence (Y.Epelboin, Acta Cryst.A,1979 35,38-44) by computing the repartition of intensity in the Borrmann fan.
Since the computation is based on the integration of the Takagi-Taupin equations, it takes into account both curved wave fields corresponding to the Eikonal theory or geometrical optics and the diffraction or newly created wavefields.
We have simulated the situation for various positions of the core of a dislocation, where it crosses the incidence plane. The images have been drawn on a color picture system, using false colors to show the different levels of intensity. They are presented in a sequence which gives the impression of a movement, as if the dislocation was moving in the crystal. This animation, in conjunction with the use of colors, allows to follow the changes in the interaction between the wave fields and the defects when its position changes in the crystal.
It shows that the interaction is much stronger when the dislocation lies near to the refracted direction and that the position of the extinction fringes is already disturbed when the dislocation crosses the incidence plane far outside the Borrmann fan, but on the side of the refracted direction. The interaction decreases very rapidly when the dislocation moves outside the Borrmann fan, on the side of the reflected direction. When the defect crosses the refracted direction, the formation of the direct image is clearly visible.
When the dislocation lies inside the Borrmann fan, we found that the position of the extinction fringes is only modified at depths greater than the position of the core of the defect. This may be explained using the notion of wave packet (F.Balibar and C.Malgrange, Acta Cryst.A, 1975, 31, 425-434): it is necessary that the wave fields travel on a distance of the order of their modulation, i.e. the extinction distance Λ, to interfere with the distorted crystal.
The formation of the intermediary image of a defect is also clearly shown: the interaction is much stronger when the dislocation crosses areas where the extinction fringes present a maximum of intensity; thus, when the depth of a defect changes the intensity of the diffracted beam oscillates, giving rise to a set of fringes whose period is roughly the same than the extinction fringes.
This short movie summarises various situations where a defect interacts with the diffracted beam in a nearly perfect crystal. The animation is a very powerful means to understand the influence of a given parameter. In the present case we have shown the influence of the position of a dislocation in the formation of its contrast.